Path Integral Invariance under Point Transformations

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We give here a covariant definition of the path integral formalism for the Lagrangian, which leaves a freedom to choose anyone of many possible quantum systems that correspond to the same classical limit without adding new potential terms nor searching for a strange measure, but using as a framework the geometry of the spaces considered. We focus our attention on the set of paths used to join succesive points in the discretization if the time-slicing definition is used to calculate the integral.If this set of paths is not preserved when performing a point transformation, the integral may change. The reasons for this are geometrically explained. Explicit calculation of the Kernel in polar coordinates is made, yielding the same system as in Cartesian coordinates.

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It has been argued that point transformations performed by simply changing integration variables in the path integral lead to inequivalent results. For example Edwards and Gulyaev [1] had shown that the free particle path integral in Cartesian coordinates is not equal to the naive expresion in polar coordinates.

This result is also quoted by several authors [2–7], who argued that new terms should be added to the action in the new coordinates beyond what would be expected clasically. The same is pointed out in the book of R.J. Rivers [8] , tracing the problem to the stochastic nature of quantum paths.

The difference between the results was explained by assuming that different orderings were given to the Hamiltonian operator in each case. This result suggests that the quantum theory inevitably depends on the choice of coordinates. While there is no guarantee that quantum mechanics should respect a classical feature such as general covariance, it is hard to believe that a physical result should depend on the coordinates used to parametrize the states. Following this philosophy, DeWitt [9] developed a covariant quantization method showing that there exists a way of changing coordinates without the system being changed. What we do here is to develop a covariant definition of the path integral that leaves a freedom to choose one from many possible quantum system that correspond to the same classical limit.

Consider the following definition for the path integral in Cartesian coordinates in two dimensions [10,11]

$$K(b,a) = \lim_{\epsilon \to 0} \frac{1}{A^{2n}} \int \cdots \int e^{\frac{i}{\hbar} S[b,a]}\, dx_1 dy_1 \ldots dx_{n-1} dy_{n-1}, \tag{1}$$

where

$$S[b,a] = \sum_{k=1}^{n} S_{cl}[x_k, y_k, t_k; x_{k-1}, y_{k-1}, t_{k-1}]. \tag{2}$$

In this last expression, S_{cl} is the classical action evaluated for a path connecting x_{k-1}, y_{k-1} and x_k, y_k (micropath), and $[b,a]$ represent the end points $(\vec{x}_b, t_b; \vec{x}_a, t_a)$. The time interval $T = t_b - t_a$ is divided into n intervals of length $\epsilon = T/n$, the integration is over all the possible positions taken at each time and $A = \left(\frac{2\pi i \hbar \epsilon}{m}\right)^{1/2}$ is the normalizing constant. Finally, the limit is taken.

The assignment $\phi[x(t)] = e^{\frac{i}{\hbar}\int \mathcal{L}(\dot{x},x,t)\, dt} = e^{\frac{i}{\hbar} S[x(t)]}$ might lead one to think that only the Lagrangian is needed to carry out the calculation of the path integral in Cartesian coordinates. However, this is not true because for non differentiable paths $\dot{x}$ doesn't exist and thus the Lagrangian is ill-defined. These paths are important because they give the largest contribution to the path integral [11]. Therefore, for these non-differentiable paths the number assigned to them may be calculated in the following way:

$$S[x(t)] = \lim_{\epsilon \to 0} \sum_{k=1}^{n} S_{cl}[x(t_a + k\epsilon), x(t_a + (k-1)\epsilon], \tag{3}$$

where

$$S_{cl}[x(t_a + k\epsilon), x(t_a + (k-1)\epsilon)] = \int_{t_a + (k-1)\epsilon}^{t_a + k\epsilon} \mathcal{L}(\dot{\psi}_k, \psi_k, t)\, dt, \tag{4}$$

here $\psi_k(t)$ describes the micropath selected to join $x(t_a+(k-1)\epsilon)$ to $x(t_a+k\epsilon)$.

We can see here that for defining the path integral one needs not only the Lagrangian but also a set of paths to join points of the discretized trajectory. This gives one the freedom of choosing different ones, which may lead to inequivalent quantum systems.

For example, consider the Lagrangian in one dimension, $\mathcal{L}=\sqrt{1+\dot{x}^2}$, which describes a free particle, and the path $x(t)\equiv 0$ from $t=0$ to $t=l$.We want to know which value will be asigned to this path. If one chooses for the ψ_k straight lines and calculate $S[x(t)]$ by limiting procedure (3) one finds $\phi[x(t)]=e^{\frac{i}{\hbar}l}$. But, if for the ψ_k one chooses semicircles and you do limiting procedure (3) one finds $\phi[x(t)]=e^{\frac{i}{\hbar}\pi l/2}$ (see FIG.1).

Now, in this example we picked up the simplest of all paths, a straight line, and with two different limiting procedures, we found two different values. The reason for this is that with straight lines, semicircles or any other kind of paths, we can approximate pointwise to the original path, but not necesarilly the derivatives have to converge to the derivatives of the original path. So, on a diferentiable path, one could say that a "good" way to calculate $S[x(t)]$ is to choose paths ψ_k that in the limit will approximate not only pointwise but also on the derivatives. But a bigger problem arises on the non-differentiable paths, because there we can't define a "good" way, and the value given to the path $x(t)$ depends exclusively on which paths ψ_k we select. So here one can clearly see that care must be taken about which micropath one chooses. In [10],pg. 34, it says "It is possible to define the path in a somewhat more elegant manner. Instead of straight lines between the points i and $i+1$, we could use sections of the classical orbit. ". But we can see in our example that changing the micropaths may change the final result, if it is not done with care. And although Feynmann introduces this to win in elegance, one can reintroduce elegance simply by defining the "straight line" as a geodesic.

Now, when a change of variables is made, one must preserve the paths ψ_k used to join the points in the discretization, because if one doesn't do that the values assigned to a specific path will change and the final result will differ. The paths are geometric objects independent of the coordinates and this is the basis of our covariant aproach. This includes choosing geodesics in the configuration space, or the classical paths, as the ψ_k. Later we show how to calculate in polar coordinates the kernel of the free particle, giving the same result as in Cartesian, with the condition that one doesn't change the values given to the paths or, what is the same, the ψ_k selected are the same.

There is another source of confusion when evaluating a path integral. Consider for instance the free particle in Cartesian coordinates; it can be shown [12] that if the Weyl ordering is considered the kernel of the Schrodinger equation can be written as:

$$K(b,a)=\lim_{\epsilon\to 0}\frac{1}{A^{2n}}\int\cdots\int e^{\frac{i}{\hbar}\sum_{k=1}^{n}\left[(x_k-x_{k-1})^2/\epsilon+(x_k-x_{k-1})^2/\epsilon-\epsilon V((x_k+x_{k-1})/2,(y_k+y_{k-1})/2)\right]}dx_1dy_1\ldots dx_{n-1}dy_{n-1}. \quad (5)$$

This expresions, however, may be wrong if we consider another ordering or curvilinear coordinates. This expression is called the mid-point definition. There are other common definitions known in literature as left or right-point which are studied by Feynman [11]. This definitions are not equivalent but they may yield the same result if the conditions discussed below are fulfilled.

In general $S_{cl}[x_k,y_k;x_{k-1},y_{k-1}]$ can be approximated so long as the error is of order $\epsilon^{1+\alpha}$ with $\alpha>0$, i.e., if a function $\bar{S}[x_k,y_k;x_{k-1},y_{k-1}]$ can be defined such that

$$S_{cl}[x_k,y_k;x_{k-1},y_{k-1}]=\bar{S}[x_k,y_k;x_{k-1},y_{k-1}]+O(\epsilon^{1+\alpha}) \quad (6)$$

calculated as (1) replacing S_{cl} by $\bar{S}$ in (2). With this result, and starting from the path integral formalism (without mentioning an order in the Hamiltonian operator), result (5) may be also understood: if we choose as micropaths the straight lines, the integral of the Lagrangian through this micropaths can be approximated by the expression on the exponent in (5) with an error $O(\epsilon^2)$ by the paralelogram law. So we can associate the Weyl ordering in Cartesian coordinates with this selection of micropaths.

So, talking about the mid-point definition (5) of path integrals can be misleading. The integral doesn't change if one chooses the right, or left, or midpoint definition while condition (6) is satisfied; they are only a tool for calculation. Any of these may be used as defining the path integral, because they provide one with a function that gives a number when you have two points in the discretized path, and so one can proceed in the calculation, but they will not agree with (5) if condition (6) is not satisfied.

Consider the kernel of the free particle in polar coordinates. The explicit expresion reads

$$K(b,a)=\frac{1}{A^2}\lim_{\epsilon\to 0}\int_0^\infty r_1\frac{dr_1}{A}\cdots\int_0^\infty r_{n-1}\frac{dr_{n-1}}{A}\int_0^{2\pi}\frac{d\theta_1}{A}\cdots\int_0^{2\pi}\frac{d\theta_{n-1}}{A}\exp\left[\frac{i}{\hbar}S(b,a)\right]. \quad (7)$$

The action can be decomposed into the sum of the actions for each segment of path. For every one of such pieces the action must be evaluated on a prescribed trajectory. We choose these trajectories to be the classical ones (straight lines) and in polar coordinates this gives the action for the total path as

$$\exp\left[\frac{i}{\hbar}S_{cl}(b,a)\right]=\prod_{k=1}^{n-1}\exp\left[\frac{im}{2\hbar\epsilon}(r_k^2+r_{k-1}^2-2r_kr_{k-1}\cos(\theta_k-\theta_{k-1})\right]. \tag{8}$$

Note that the micropaths choosen are the geodesics in the polar plane, that in this case coincides with the classic trajectory of the particle; we don't need to know what was the result of quantization in Cartesian: we only need the Lagrangian and the geometry of the new coordinates. As we go over the paths, $\theta_k-\theta_{k-1}$ need not to be small. This difference can take all values between 0 and 2π, so one can't expand the cosine and keep only the lowest order terms as is done in [1]. In order to calculate the kernel we first collect the terms in an integral of the general form $\int_0^{2\pi}\exp\left[i(C\cos\theta+S\sin\theta)\right]\,d\theta$ which can be readily done by integrating over the unit circle in the complex plane and calculating the residues. The result is $\frac{2\pi}{A}J_0(\sqrt{C^2+S^2})$, where J_0 is the Bessel function of the first kind of order 0. Next we collect the terms in r_1 obtaining an integral that can be worked out using the following result [13]

$$\int_0^\infty x^{\nu+1}e^{\pm i\alpha x^2}J_\nu(\beta x)\,dx=\frac{\beta^\nu}{(2\alpha)^{\nu+1}}\exp\left[\pm i\left(\frac{\nu+1}{2}\pi-\frac{\beta^2}{4\alpha}\right)\right] \tag{9}$$

where $\alpha\,,\beta\;>\;0$ and $-1\;<\;Re(\nu)\;<\;1/2$. Using this formula with $\nu\;=\;0$, $\alpha\;=\;m/\hbar\epsilon$ and $\beta\;=\;(m/\hbar\epsilon)\sqrt{r_0^2+r_2^2+2r_0r_2\cos(\theta_2-\theta_0)}$, gathering all the terms in $r_0\,,r_2$ and replacing the apropriate constants we obtain the integrals over r_1 and θ_1 and continuing with this process after $n-1$ integrations we obtain

$$\frac{1}{n}\exp\left(\frac{im}{n\hbar\epsilon}\left(\frac{n+1}{2}r_n^2+\frac{1}{2}r_0^2-r_nr_0\cos(\theta_n-\theta_0)\right)\right). \tag{10}$$

We have to multiply now by the term $\exp(-imr_n^2/2\hbar\epsilon)$, because we were multipliyng each time by $\exp(imr_k^2/\hbar\epsilon)$, but because r_n is an end point we have only $\exp(imr_n^2/2\hbar\epsilon)$. So, using the fact that $n\epsilon=T=t_b-t_a$ we finally obtain for the kernel in polar coordinates:

$$K(b,a)=\frac{m}{2\pi\hbar Ti}\exp\left[\frac{im}{2T\hbar}\left(r_n^2+r_0^2-2r_nr_k\cos(\theta_n-\theta_k)\right)\right]. \tag{11}$$

This result is the same as the standard one in Cartesian coordinates [10] making the substitution $x=r\cos\theta$, $y=r\sin\theta$.This result is clear from (7). Thus, we have shown that, under the constrain of mantaining the paths ψ_k that join points in the discretization

$$\int\mathcal{D}x\mathcal{D}y\exp\left(\frac{i}{\hbar}\int\,dt\left(\frac{1}{2}(\dot{x}^2+\dot{y}^2)\right)\right)=\int\mathcal{D}r\mathcal{D}\theta J[r]\exp\left(\frac{i}{\hbar}\int\,dt\left(\frac{1}{2}(\dot{r}^2+r^2\dot{\theta}^2)\right)\right), \tag{12}$$

where the regularization used is understood.

Explicit application of the conservation of micropaths to define a covariant path integral may be found in [14,15] for curved configuration space using the geodesics as micropaths. For phase space, there is a very clear exposition for point canonical and other transformations in [16].

Point transformations can be made in the naive way so long as the micropaths between two points in the discretization is preserved. One needs not add extra potential terms to the classsical Lagrangian when changing coordinates, nor search for strange measures in order to get the correct result—which just means getting the same result as in the original integral. Different orderings in the Hamiltonian operator may be related to the different choices in the paths that join two points of the discretization, because this is one of the freedoms in the definition of the path integral. This freedom is unrelated whatsoever to that of choosing another set of coordinates in the Lagrangian to represent the same system. Another freedom is to choose an equivalent Lagrangian for the system.

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FIG. 1. In this figure we can see the limiting procedure with which we approximate the straight line with semicircles.

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